Stability theory for difference approximations of some dispersive shallow water equations and application to thin film flows

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Abstract

In this paper, we study the stability of various difference approximations of the Euler-Korteweg equations. This system of evolution PDEs is a classical isentropic Euler system perturbed by a dispersive (third order) term. The Euler equations are discretized with a classical scheme (e.g. Roe, Rusanov or Lax-Friedrichs scheme) whereas the dispersive term is discretized with centered finite differences. We first prove that a certain amount of numerical viscosity is needed for a difference scheme to be stable in the Von Neumann sense. Then we consider the entropy stability of difference approximations. For that purpose, we introduce an additional unknown, the gradient of a function of the density. The Euler-Korteweg system is transformed into a hyperbolic system perturbed by a second order skew symmetric term. We prove entropy stability of Lax-Friedrichs type schemes under a suitable Courant-Friedrichs-Levy condition. We validate our approach numerically on a simple case and then carry out numerical simulations of a shallow water system with surface tension which models thin films down an incline. In addition, we propose a spatial discretization of the Euler-Korteweg system seen as a Hamiltonian system of evolution PDEs. This spatial discretization preserves the Hamiltonian structure and thus is naturally entropy conservative. This scheme makes possible the numerical simulation of the dispersive shock waves of the Euler Korteweg system.

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1 Introduction

This paper is motivated by the numerical simulation of the so-called Euler-Korteweg system, which arises in the modelling of capillary fluids: these comprise liquid-vapor mixtures (for instance highly pressurized and hot water in nuclear reactors cooling system, in which the presence of vapor is actually dramatic), superfluids (Helium near absolute zero), or even regular fluids at sufficiently small scales (think of ripples on shallow water or other thin films). In one space dimension, the most general form of the Euler-Korteweg system we consider is

$$\begin{aligned} &\partial_t\rho + \partial_x(\rho u) = 0, \\ &\partial_t(\rho u) + \partial_x\left(\rho u^2 + P(\rho)\right) = \partial_x\left(\rho\kappa(\rho)\partial_{xx}\rho + (\rho\kappa'(\rho) - \kappa(\rho))\frac{(\partial_x\rho)^2}{2}\right), \end{aligned} \tag{1.1}$$

where ρ denotes the fluid density, u the fluid velocity, $P(\rho)$ the fluid pressure and $\kappa(\rho)$ the capillary coefficient. In quantum hydrodynamics, the capillary coefficient is chosen so that $\rho\kappa(\rho) = \textit{constant}$ whereas for classical applications, like thin film flows, it is often chosen to be constant. In particular, we will focus, for numerical computations, to the case of thin film flows down an incline modeled by the shallow water equations with surface tension and source term

$$\begin{aligned} &\partial_t h + \partial_x(hu) = 0, \\ &\partial_t(hu) + \partial_x\left(hu^2 + P(h, A_1)\right) = A_1\left(gh\sin(\theta) - 3\frac{\nu u}{h} + \frac{\sigma}{\rho}h\partial_{xxx}h\right), \end{aligned} \tag{1.2}$$

where h is the fluid height, u the streamwise velocity averaged along the cross stream direction. The constant ρ, ν, σ are respectively the density, viscosity and capillarity of the fluid used in the Liu-Gollub experiment [LG] whereas g is the constant of gravity and θ is the slope of the channel. The constant $A_1 > 0$ is arbitrary and $P(h, A_1)$ is a smooth pressure term.

The Euler-Korteweg system (1.1) falls in the class of abstract Hamiltonian systems of evolutions PDEs when it is written with variables ρ, u:

$$\partial_t U = \mathcal{J}\left(\mathrm{E}\mathcal{H}[U]\right), \tag{1.3}$$

with $U = (\rho, u)^T$, $\mathcal{J} = \partial_x \mathrm{J}$,

$$\mathrm{J} = \begin{pmatrix} 0 & -1 \\ -1 & 0 \end{pmatrix}, \quad \mathcal{H}[U] = \frac{\rho u^2}{2} + F(\rho) + \kappa(\rho)\frac{(\partial_x\rho)^2}{2} = \frac{\rho u^2}{2} + \mathcal{E}(\rho, \partial_x\rho),$$

and E denotes the Euler operator

$$\mathrm{E}\mathcal{H}[U] = \begin{pmatrix} \frac{u^2}{2} + F'(\rho) + \kappa'(\rho)\frac{(\partial_x\rho)^2}{2} - \partial_x(\kappa(\rho)\partial_x\rho) \\ \rho u \end{pmatrix} = \begin{pmatrix} \frac{u^2}{2} + \mathrm{E}_\rho\mathcal{E}(\rho, \partial_x\rho) \\ \rho u \end{pmatrix}.$$

The pressure P is related to F through the relation $\rho F'(\rho) - F(\rho) = P(\rho)$. Due to the invariance of the equations with respect to spatial translations and time translations, the system (1.3) admits, via Noether's theorem, two additional conservation laws which are nothing but the conservation of momentum (and the second equation of (1.1)) and the conservation of energy:

$$\partial_t(\rho u) + \partial_x\left(\rho u^2 + P(\rho)\right) = \partial_x\left(\rho\kappa(\rho)\partial_{xx}\rho + (\rho\kappa'(\rho) - \kappa(\rho))\frac{(\partial_x\rho)^2}{2}\right),$$

$$\partial_t\left(\frac{1}{2}\rho u^2 + \mathcal{E}(\rho, \partial_x\rho)\right) + \partial_x\left(\frac{1}{2}\rho u^3 + \rho u \mathrm{E}_\rho\mathcal{E}(\rho, \partial_x\rho) + \kappa(\rho)\partial_x(\rho u)\partial_x\rho\right) = 0. \tag{1.4}$$

As a consequence, when the system (1.1) is set on the real line or with periodic boundary conditions, the energy (here the Hamiltonian $\mathcal{H}$) is conserved. Therefore, it is desirable from a numerical point of view that a difference approximation of (1.1) or (1.3) preserves the energy or, at least, dissipates energy. In the first case, the difference approximation is an “entropy conservative” scheme and in the later case, it is an “entropy stable” scheme.

At this stage, there are two possible strategies to tackle this problem. The first one consists in considering the system (1.1) as a dispersive perturbation of the classical isentropic Euler equations. This is the point of view adopted e.g. in [LMR]. Here the authors construct fully discrete entropy conservative scheme for systems of conservation laws (hyperbolic or hyperbolic-elliptic) endowed with an entropy-entropy flux pair. These difference approximations are second and third order accurate and can in turn be used to construct a numerical method for the computation of weak solutions containing non- classical regularization-sensitive shock waves. In particular, the authors considered dissipative/dispersive regularizations that are linear in the entropy variables

$$\partial_t u(v^\varepsilon) + \partial_x f(u(v^\varepsilon)) = \varepsilon B_2 \partial_{xx} v^\varepsilon + \varepsilon^2 B_3 \partial_{xxx} v^\varepsilon, \quad 0 < \varepsilon \ll 1$$

with B_i constant matrices, B_2 being positive definite and B_3 symmetric. Therefore the dispersive terms do not contribute in the energy equation:

$$\partial_t \int_{\mathbb{R}} U(u^\varepsilon) \leq 0.$$

where U is the entropy associated to the system of conservation laws

$$\partial_t u + \partial_x f(u) = 0.$$

This situation contrasts with the one met in the Euler-Korteweg system where the dispersive terms have a contribution in the energy balance

$$\partial_t \int_{\mathbb{R}} \left(\frac{1}{2}\rho u^2 + F(\rho)\right) + \kappa(\rho)\frac{(\partial_x \rho)^2}{2} = 0.$$

As a consequence, an entropy conservative or entropy stable scheme for the isentropic Euler equations coupled with a centered approximation of dispersive terms may not provide an entropy conservative nor entropy stable scheme for the Euler-Korteweg system. This issue was considered in [CL] where Euler Kortweg equations are written in lagrangian coordinates of mass: by introducing an extended formulation of the system, the authors derived a family of high order and entropy conservative semi-discrete schemes. With these high order approximations schemes in hand, the authors then computed kinetic relations for Van der Waals fluids. Though, the lagrangian coordinates of mass can not be used in dimension d with $d \geq 2$ and one has to consider an alternative extended formulation in Eulerian coordinates: this latter point of view will be expanded here, based on the extended formulation found in [BDD, BDDd].

In section 2, we consider the stability of various difference approximations of Euler-Korteweg equations in the Von Neumann sense. We shall prove that even at that linear level, the Godunov scheme (explicit and implicit in time) is always unstable. In this direction, we checked the stability of Lax-Friedrichs type schemes: we show that it is stable in the Von Neumann sense under a suitable Courant-Friedrichs-Levy (CFL) condition for explicit forward Euler (resp. Runge Kutta) time discretization for first order (resp. second order) difference schemes. This analysis provides necessary conditions of stability for the simulations of the fully nonlinear system. Finally we show that the implicit backward Euler time discretization is always stable.

In section 3, we move to the entropy (nonlinear) stability problem. It is a hard problem to obtain directly entropy stability from nonlinear difference approximation of Euler Korteweg equations since discrete integration by parts and time discretization do not commute. Here, we introduce an additional variable $w = \sqrt{\kappa(\rho)}\partial_x\rho/\sqrt{\rho}$ and derive a conservation law for w. In this new formulation, the capillary term appears as an anti dissipative term in the system for (u, w) and one can prove the well-posedness of the Euler-Korteweg system [BDD]. Moreover, the derivation of the energy estimate follows the same line as a classical energy estimate in the isentropic Euler equations. In that setting, we show difference approximations made of a Lax-Friedrichs (entropy stable) scheme for the hyperbolic part and centered difference for the anti-diffusive part is entropy stable under a suitable CFL condition for explicit forward Euler time discretization and always stable for implicit backward Euler time discretization.

Finally, in section 4, we carry out numerical simulations of shallow water equations with surface tension. We first consider thin film flow over a flat bottom and neglect source terms so as to compare entropy stability of difference approximations for shallow water in original form and for its new formulation counterpart. The numerical simulations clearly show that the discretization of new formulation of shallow water equations has better entropy stability property.

Then, we introduce a difference approximation of the shallow water equations written as a Hamiltonian system of evolution PDEs. The semi discretized system is Hamiltonian and trivially preserves a discrete Hamiltonian that is consistent with the continuous one. Then, one is left with the problem of time discretization: the explicit forward Euler is always unstable and one has to consider implicit time discretization to obtain an entropy stable scheme: the numerical simulation of this Hamiltonian system shows that the dynamical behavior is completely changed in comparison to entropy stable schemes. Indeed, this Hamiltonian difference approximation has no numerical viscosity, so that one can observe the formation of so called "dispersive shock waves" [E, EGK, EGS]. Here, the classic hyperbolic shocks are regularized by dispersive effects and an oscillatory zone appear and grows with time. We conclude this section with numerical simulation of a Liu Gollub experiment [LG] modeled by a consistent shallow water model with source term derived in [NV].

2 Von Neumann stability of difference schemes

In this section, we linearize the Euler-Korteweg system about constant states and study the Von Neumann-stability of various difference approximations. We have first considered two classes of spatial discretisations, namely Godunov and Lax-Friedrichs type schemes for the first part of the equations whereas the dispersive term is discretized with classical centered difference approximations. We prove that the Godunov scheme is always unstable both with explicit forward and implicit backward Euler time discretization. The Lax-Friedrichs type schemes inherit better stability properties: we prove that it is stable under a CFL condition for explicit forward Euler time discretization and always stable for implicit backward Euler time discretization.These difference approximations are first order accurate in time and space: we have also considered second order accurate schemes, namely MUSCL scheme with a Lax-Friedrichs flux. We prove the stability of explicit Runge Kutta (second order accurate) time integration under a CFL condition and stability of Crank-Nicolson time discretization.

The linearized Euler-Korteweg equations (in $(\rho, q = \rho u)$ variables) are given by

$$\partial_t \rho + \partial_x q = 0, \quad \partial_t q + (\bar{c}^2 - \bar{u}^2)\partial_x \rho + 2\bar{u}\partial_x q = \bar{\sigma}\partial_{xxx}\rho, \tag{2.1}$$

with $\bar{\sigma} = \bar{\rho}\kappa(\bar{\rho})$. With Riemann invariants, this system is also written as

$$\partial_t r + (\bar{u} - \bar{c})\partial_x r = -\bar{\sigma}\partial_{xxx}(r+s), \quad \partial_t s + (\bar{u} + \bar{c})\partial_x s = \bar{\sigma}\partial_{xxx}(r+s). \tag{2.2}$$

2.1 Instability of Godunov type schemes

In this section, we consider Godunov schemes for the hyperbolic part of the equations and centered finite difference approximation of the third order partial derivative. In order to simplify the analysis, we deal with a diagonalized version of the first order part (2.2). Let us introduce the matrices A and B

$$A = \begin{pmatrix} \bar{u} - \bar{c} & 0 \\ 0 & \bar{u} + \bar{c} \end{pmatrix}, \quad B = \begin{pmatrix} -\bar{\sigma} & -\bar{\sigma} \\ \bar{\sigma} & \bar{\sigma} \end{pmatrix}$$

so that, by setting $v = (r, s)^T$, the system (2.2) reads

$$\partial_t v + A\partial_x v = B\partial_{xxx} v. \tag{2.3}$$

We first consider supersonic flows $\bar{u} > \bar{c} > 0$: the Godunov scheme reads

$$\frac{dv_j}{dt} + A\frac{v_j - v_{j-1}}{\delta x} = B\frac{v_{j+2} - 2v_{j+1} + 2v_{j-1} - v_{j-2}}{2\delta x^3}, \quad i \in \mathbb{Z}. \tag{2.4}$$

Then the explicit forward Euler (FE) and implicit backward Euler (BE) read

$$v_j^{n+1} - v_j^n + \lambda_1 A(v_j^n - v_{j-1}^n) = \frac{\lambda_3}{2} B\left(v_{j+2}^n - 2v_{j+1}^n + 2v_{j-1}^n - v_{j-2}^n\right), \tag{2.5}$$

$$v_j^{n+1} - v_j^n + \lambda_1 A(v_j^{n+1} - v_{j-1}^{n+1}) = \frac{\lambda_3}{2} B\left(v_{j+2}^{n+1} - 2v_{j+1}^{n+1} + 2v_{j-1}^{n+1} - v_{j-2}^{n+1}\right), \tag{2.6}$$

where $\lambda_k = \delta t/\delta x^k$ encode the classical CFL conditions for hyperbolic equations ($k = 1$), parabolic equations ($k = 2$) and dispersive equations ($k = 3$). We prove the following proposition.

Proposition 2.1. *Assume $\bar{u} > \bar{c} > 0$, there exist $\Lambda > 0$ and $h > 0$ such that if $0 < \lambda_3 < \Lambda$ and $0 < \delta x < h$ then the difference approximations (2.5) and (2.6) of the linearized Euler-Korteweg system are unstable in the Von Neumann sense.*

Proof. Let us start with the explicit forward Euler time discretization: we search for solution of (2.5) in the form $v_j^n = X^n e^{-ij\xi}\hat{v}$. Then, $(X, \hat{v})$ satisfies the spectral problem

$$\begin{aligned} X\hat{v} &= \begin{pmatrix} 1 + \lambda_1\delta(\xi)(\bar{u} - \bar{c}) - i\bar{\sigma}\gamma(\xi)\lambda_3 & -i\bar{\sigma}\gamma(\xi)\lambda_3 \\ i\bar{\sigma}\gamma(\xi)\lambda_3 & 1 + \lambda_1\delta(\xi)(\bar{u} + \bar{c}) + i\bar{\sigma}\gamma(\xi)\lambda_3 \end{pmatrix}\hat{v} \\ &= M_2(\xi, \lambda_1, \lambda_3)\hat{v}, \end{aligned}$$

with $\delta(\xi) = e^{i\xi} - 1$ and $\gamma(\xi) = 4\sin(\xi)(1-\cos(\xi))$. Hence X lies in $\mathrm{Sp}(M_2(\xi, \lambda_1, \lambda_3))$ and satisfies the following equation:

$$(X-1)^2 - 2\lambda_1\delta(\xi)\bar{u}(X-1) - 2i\bar{\sigma}\bar{c}\gamma(\xi)\delta(\xi)\lambda_1\lambda_3 + O(\lambda_1^2) = 0.$$

Recall that $\lambda_1 = \lambda_3\delta x^2$. Next, we expand X with respect to $0 < \lambda_3 \ll 1$ and $0 < \delta x \ll 1$: for that purpose, we set $X = 1 + \lambda_3\delta x\tilde{X}$. Then, one has

$$\tilde{X}^2 - 2i\bar{\sigma}\bar{c}\gamma(\xi)\delta(\xi) = 2\delta(\xi)\bar{u}\,\delta x + O(\delta x^2),$$

where $O(\delta x^2)$ denotes a smooth function of δx, independent of λ_i and of order $O(\delta x^2)$. Then, we choose $\xi = \pi/2$: by a classic application of the implicit function theorem, one obtains that $X \in \mathrm{Sp}(M_2(\pi/2, \lambda_1, \lambda_3))$ expands as

$$X = 1 \pm 4\sqrt{\bar{\sigma}\bar{c}\cos(\pi/4)}e^{i\frac{\pi}{8}}\lambda_3\delta x + O(\lambda_3\delta x^2).$$

As a result, one finds

$$|X|^2 = 1 \pm 8\sqrt{\bar{\sigma}\bar{c}\cos(\pi/4)}\cos(\pi/8)\lambda_3\delta x + O(\lambda_3\delta x^2).$$

Then, for λ_3 and δx sufficiently small, $M_2(\pi/2, \lambda_1, \lambda_3)$ has two eigenvalues $X_\pm$ such that $|X_-| < 1 < |X_+|$ and the explicit in time Godunov scheme is unstable in the Von Neumann sense.

The instability of the implicit Godunov scheme then follows easily. Indeed, by searching for solutions of (2.6) in the form $v_j^n = X^n e^{-ij\xi}\hat{v}$, one obtains the spectral problem

$$X\hat{v} = M_2(\xi, -\lambda_1, -\lambda_3)^{-1}\hat{v} = M_3(\xi, \lambda_1, \lambda_3)\hat{v},$$

and it is easily seen that for λ_3 and δx sufficiently small, $M_3(\pi/2, \lambda_1, \lambda_3)$ has two eigenvalues $X_\pm$ so that $|X_-| < 1 < |X_+|$ and the implicit in time Godunov scheme is unstable. □

Remark 2.2. *This instability can be explained by the fact that for the continuous system the flow is not always supercritical. Indeed, searching for solutions of the continuous system* (2.1) *in the form* $(\rho, q) = e^{ik(x-st)}(\hat{\rho}, \hat{q})$, *one finds*

$$s_\pm(k) = \bar{u} \pm \sqrt{\bar{c}^2 + \bar{\sigma}k^2}.$$

Then, if $|k| < k_c = \sqrt{(\bar{u}^2 - \bar{c}^2)/\bar{\sigma}}$, *the flow is supercritical :*$0 < s_-(k) < s_+(k)$ *whereas for sufficiently large wavenumbers* $|k| > k_c$, *the flow is subcritical:* $s_-(k) < 0 < s_+(k)$. *As a consequence an upwind strategy necessarily fails: instability is found for wave trains with large wave number (or equivalently for small* δx*).*

Though, even in the subcritical case $0 < \bar{u} < \bar{c}$ where the flow remains subcritical when the dispersive term is added ($s_-(k) < 0 < s_+(k)$, $\forall k \in \mathbb{R}$), the Godunov scheme is unstable. We prove the following proposition.

Proposition 2.3. *For subcritical flows, $0 < \bar{u} < \bar{c}$, there exists $\Lambda > 0$ and $h > 0$ such that if $0 < \lambda_3 < \Lambda$ and $0 < \delta x < h$ then the Godunov space discretization yields an unstable scheme in the Von Neumann sense for both explicit forward and implicit backward Euler time discretization.*

Proof. The semi discretized Godunov scheme is written as

$$\begin{pmatrix} \dfrac{dr_j}{dt} + (\bar{u} - \bar{c})\dfrac{r_{j+1} - r_j}{\delta x} \\ \dfrac{ds_j}{dt} + (\bar{u} + \bar{c})\dfrac{r_j - r_{j-1}}{\delta x} \end{pmatrix} = B\frac{v_{j+2} - 2v_{j+1} + 2v_{j-1} - v_{j-2}}{2\delta x^3}.$$

We use the notations introduced in the proof of proposition 2.1. Let us first consider the explicit forward Euler time discretization. In this case, the spectral problem reads

$$\begin{aligned} X\hat{v} &= \begin{pmatrix} 1 + \lambda_1 \overline{\delta(\xi)}(\bar{c} - \bar{u}) - i\bar{\sigma}\gamma(\xi)\lambda_3 & -i\bar{\sigma}\gamma(\xi)\lambda_3 \\ i\bar{\sigma}\gamma(\xi)\lambda_3 & 1 + \lambda_1\delta(\xi)(\bar{u} + \bar{c}) + i\bar{\sigma}\gamma(\xi)\lambda_3 \end{pmatrix}\hat{v} \\ &= \tilde{M}_2(\xi, \lambda_1, \lambda_3)\hat{v}. \end{aligned}$$

Then X lies in $\mathrm{Sp}(\tilde{M}_2(\xi, \lambda_1, \lambda_3))$ and satisfies

$$\begin{aligned} (X-1)^2 - \lambda_1(\overline{\delta(\xi)}(\bar{c} - \bar{u}) + \delta(\xi)(\bar{u} + \bar{c}))(X - 1) \\ + i\bar{\sigma}\lambda_1\lambda_3\gamma(\xi)\left(\overline{\delta(\xi)}(\bar{c} - \bar{u}) - \delta(\xi)(\bar{u} + \bar{c})\right) + O(\lambda_1^2) = 0. \end{aligned}$$

By setting $X = 1 + \lambda_3 \delta x \tilde{X}$, one obtains

$$\tilde{X}^2 + i\bar{\sigma}\gamma(\xi)\left(\overline{\delta(\xi)}(\bar{c} - \bar{u}) - \delta(\xi)(\bar{u} + \bar{c})\right) = \delta x(\overline{\delta(\xi)}(\bar{c} - \bar{u}) + \delta(\xi)(\bar{u} + \bar{c}))\tilde{X} + O(\delta x^2).$$

This is also written as

$$\tilde{X}^2 + 2\bar{\sigma}\gamma(\xi)\left(i\bar{u}(1 - \cos(\xi)) + \bar{c}\sin(\xi)\right) = O(\delta x).$$

Let us choose $\xi = \pi/2$: then, it is easily proved that $X \in \sigma(\tilde{M}_2(\pi/2, \lambda_1, \lambda_3))$ expands as

$$X = 1 \pm 4\sqrt{\bar{\sigma}\bar{c}\cos(\pi/4)}e^{i\dfrac{\pi}{8}}\lambda_3\delta x + O(\lambda_3\delta x^2).$$

Thus, one easily finds that for λ_3 and dx sufficiently small, there are two eigenvalues $X_\pm$ so that $|X_-| < 1 < |X_+|$ and the explicit Godunov scheme is unstable.By using a similar argument, one proves easily that the implicit backward time discretization yields an unstable scheme as well. □

Remark 2.4. *The instability still arises in the subcritical case since the Riemann invariants r, s for the first order system does not always represent respectively a subcritical and supercritical mode: it depends again on the wavenumber.*

2.2 Stability of Lax-Friedrichs type schemes

In this section, we check the stability of Lax Friedrichs type scheme in the Von Neumann sense: this provides necessary, and in general, practical conditions, for the stability of the nonlinear difference approximations. Since there is no upwind strategy, we discretized directly (2.1). Let us introduce the matrices A and B

$$A = \begin{pmatrix} 0 & 1 \\ \bar{c}^2 - \bar{u}^2 & 2\bar{u} \end{pmatrix}, \quad B = \begin{pmatrix} 0 & 0 \\ \bar{\sigma} & 0 \end{pmatrix}$$

so that system (2.1) reads

$$\partial_t v + A\partial_x v = B\partial_{xxx} v. \tag{2.7}$$

2.2.1 First order accurate schemes

We first discretize in space by using centered differences for the third order derivative and a Lax Friedrichs type flux for the hyperbolic part. The semi-discretized approximation then reads

$$\begin{aligned} \frac{dv_j}{dt} &= -\frac{\triangle_+ g_{LF}(v_{j-1}, v_j)}{\delta x} + \frac{B}{2\delta x^3}(v_{j+2} - 2v_{j+1} + 2v_{j-1} - v_{j-2}) \\ &= -A\frac{v_{j+1} - v_{j-1}}{2\delta x} + \frac{Q}{2\delta t}(v_{j+1} - 2v_j + v_{j-1}) + B\frac{v_{j+2} - 2v_{j+1} + 2v_{j-1} - v_{j-2}}{2\delta x^3}, \end{aligned} \tag{2.8}$$

where $\Delta_+ v_j = v_{j+1} - v_j$ and

$$g_{LF}(u_l, u_r) = \frac{F(u_l) + F(u_r)}{2} - \frac{Q}{2\lambda_1}(u_r - u_l)$$

is a general Lax-Friedrichs flux. The classical Lax Friedrichs scheme is obtained by setting $Q = 1$, whereas if $Q = \frac{1}{2}$ one finds the modified Lax-Friedrichs scheme [T]. Finally, by setting $Q = \lambda_1 \|A\| = \lambda_1(\bar{u} + \bar{c})$, one obtains the Rusanov scheme.

We search for spatially bounded solutions of (2.8) in the form $v_j = e^{ij\xi}\hat{v}$. This yields

$$\frac{d\hat{v}}{dt} = -i\frac{\alpha(\xi)}{\delta x}A\hat{v} + \frac{Q}{2\delta t}\beta(\xi)\hat{v} = i\frac{\gamma(\xi)}{\delta x^3}B\hat{v} \tag{2.9}$$

with

$$\alpha(\xi) = \frac{e^{-i\xi} - e^{i\xi}}{2i} = -\sin(\xi), \quad \beta(\xi) = e^{-i\xi} - 2 + e^{i\xi} = 2(\cos(\xi) - 1),$$
$$\gamma(\xi) = \frac{e^{-2i\xi} - 2e^{-i\xi} + 2e^{i\xi} - e^{2i\xi}}{2i} = 2\sin(\xi) - \sin(2\xi) = 2\sin(\xi)(1 - \cos(\xi)).$$

Let us now consider various time discretizations. The forward explicit /backward implicit Euler time discretizations and θ-scheme for (2.9) are written as

- (FE) Euler: $\hat{v}^{n+1} - \hat{v}^n + (i\lambda_1\alpha(\xi)A - \frac{Q}{2}\beta(\xi)\mathrm{Id})\hat{v}^n = i\lambda_3\gamma(\xi)B\hat{v}^n$
- (BI) Euler: $\hat{v}^{n+1} - \hat{v}^n + (i\lambda_1\alpha(\xi)A - \frac{Q}{2}\beta(\xi)\mathrm{Id})\hat{v}^{n+1} = i\lambda_3\gamma(\xi)B\hat{v}^{n+1}$
- θ-Scheme: $\hat{v}^{n+1} = \hat{v}^n - \left(i\lambda_1\alpha(\xi)A - \dfrac{Q}{2}\beta(\xi)\mathrm{Id} - i\lambda_3\gamma(\xi)B\right)((1-\theta)\hat{v}^{n+1} + \theta v^n)$.

Theses difference approximations are all first order accurate both in space and time. In the particular case $\theta = 1/2$ (Crank-Nicolson time discretization), the difference approximation is second order accurate in time.

We first study the (FE) time disretization. Denote $R(Q, m, |\bar{u}|, \bar{c})$ the function

$$R(Q, m, |\bar{u}|, \bar{c}) = \min_{0 \le x \le 2} \left(\frac{2Q - Q^2 x}{(2-x)\left(|\bar{u}| + \sqrt{\bar{c}^2 + 2mx}\right)^2} \right).$$

Note that

$$R(1, m, |\bar{u}|, \bar{c}) = \frac{1}{\left(|\bar{u}| + \sqrt{\bar{c}^2 + 4m}\right)^2}.$$

We prove the following proposition.

Proposition 2.5. *The (FE) time discretization yields a stable scheme in the Von Neumann sense if and only if* $0 < Q \le 1$ *and*

$$\lambda_1^2 \le R\left(Q, \frac{\bar{\sigma}\lambda_3}{\lambda_1}, |\bar{u}|, \bar{c}\right)$$

Proof. The (FE) time discretization yields the finite difference scheme:

$$\hat{v}^{n+1} = (1 - Q(1 - \cos(\xi)))\mathrm{Id} + i\sin(\xi)M_0(\xi, \lambda_1, \lambda_3))\,\hat{v}^n$$

with $M_0(\xi, \lambda_1, \lambda_3) = \lambda_1 A + 2\lambda_3 B(1 - \cos(\xi))$. The scheme is stable in the Von Neumann sense provided that

$$\mathrm{Sp}\left(((1 - Q(1 - \cos(\xi)))\mathrm{Id} + i\sin(\xi)M_0(\xi, \lambda_1, \lambda_3))\right) \subset \{\lambda \in \mathbb{C}; |\lambda| \le 1\}.$$

By an easy computation, one shows that

$$\mathrm{Sp}\left(M_0(\xi,\lambda_1,\lambda_3)\right) = \left\{\lambda_1\left(\bar{u} \pm \sqrt{\bar{c}^2 + 2\bar{\sigma}\frac{\lambda_3}{\lambda_1}(1-\cos(\xi))}\right)\right\} = \{\lambda_1\gamma_\pm\}.$$

Let $x = 1-\cos(\xi)$: the Lax Friedrichs scheme is stable if

$$(1-Qx)^2 + \lambda_1^2 x\,(2-x)\left(|\bar{u}| + \sqrt{\bar{c}^2 + 2\bar{\sigma}\frac{\lambda_3}{\lambda_1}x}\right)^2 \leq 1.$$

A necessary condition for the stability of the finite difference scheme is $0 < Q \leq 1$. Let us now define

$$R\,(Q,m,|u|,c) = \min_{0\leq x\leq 2}\left(\frac{2Q - Q^2 x}{(2-x)\left(|u| + \sqrt{c^2+2mx}\right)^2}\right)$$

Then, the finite difference scheme is stable under the assumption $0 < Q \leq 1$ and

$$\lambda_1^2 \leq R(Q,\bar{\sigma}\frac{\lambda_3}{\lambda_1},|\bar{u}|,\bar{c}).$$

This completes the proof of the proposition. □

Corollary 2.6. *The difference approximation associated to the classical Lax-Friedrichs scheme, $Q=1$, is stable in the Von Neumann sense if and only if*

$$\lambda_1\left(|u| + \sqrt{\bar{c}^2 + \frac{4\bar{\sigma}}{\delta x^2}}\right) \leq 1 \quad (CFL)_1.$$

The difference approximation associated to the Rusanov scheme, $Q = (\bar{u}+\bar{c})\lambda_1 = \rho\lambda_1$ is stable in the Von Neumann sense if

$$\lambda_1\frac{\left(|\bar{u}| + \sqrt{\bar{c}^2 + \dfrac{4\bar{\sigma}}{\delta x^2}}\right)^2}{|\bar{u}|+\bar{c}} \leq 1.$$

Remark 2.7. *In the case of the classical Friedrichs scheme, we obtained a Courant-Friedrichs-Levy (CFL) condition for $\delta t = O(\delta x^2)$. Indeed, one can see heuristically that this condition is a necessary condition of stability. Indeed, in Fourier space, the wave speeds of (2.7) are written as $s(k) = \bar{u} \pm \sqrt{\bar{c}^2 + \bar{\sigma}k^2}$. Then, in the large wavenumber limit, one has $s(k) \leq \bar{C}|k|$. Heuristically, it is necessary for a numerical*

stable to be stable that the domain of dependence of the numerical solution contains the domain of dependence of the exact solution. This is also written as $s(k)\,\delta t/\delta x < 1$. On a spatial grid with stepsize δx, one has $s(k) \le \bar{C}/\delta x$ since the largest wavenumber is $O(1/\delta x)$. As a consequence, one obtains a heuristic CFL condition $\bar{C}\delta t/\delta x^2 < 1$ which is precisely the CFL type condition for the Lax-Friedrichs scheme. It is easily seen on the Rusanov scheme that this condition is not sufficient to get stability: here a necessary condition of stability is $\delta t = O(\delta x^3)$.

Let us now consider backward implicit Euler time discretization of (2.9):

$$(1 + Q(1 - \cos(\xi)))\mathrm{Id} - i\sin(\xi)M_0(\xi, \lambda_1, \lambda_3))\,\hat{v}^{n+1} = v^n.$$

This scheme is stable in the Von Neumann sense if and only if

$$\left(1 + Q\left(1 - \cos(\xi)\right)\right)^2 + \lambda_1^2 \sin^2(\xi)\left(|\bar{u}| + \sqrt{\bar{c}^2 + 2\bar{\sigma}\frac{\lambda_3}{\lambda_1}(1 - \cos(\xi))}\right)^2 \ge 1,$$

which, obviously, holds true for all $Q \ge 0$.

We end this section by checking the stability of θ-schemes. We prove the following proposition.

Proposition 2.8. *If $\theta > \frac{1}{2}$, the θ-scheme is stable in the Von Neumann sense if and only if*

$$(2\theta - 1)\,Q \le 1$$

with

$$(2\theta - 1)^2\,\lambda_1^2 \le R\left(Q\,(2\theta - 1)\,, \frac{\lambda_3}{\lambda_1}, |\bar{u}|, \bar{c}\right)$$

If $\theta \le \frac{1}{2}$, the θ-scheme is always stable.

Proof. The θ-scheme can be written as $\hat{v}^{n+1} = M_1(\xi, \lambda_1, \lambda_3, \theta)v^n$ and the spectrum of $M_1(\xi, \lambda_1, \lambda_3, \theta)$ is given by

$$\mathrm{Sp}(M_1(\xi, \lambda_1, \lambda_3, \theta)) = \left\{\frac{1 - \theta Q(1 - \cos(\xi)) + i\theta\sin(\xi)\lambda_1\gamma_\pm}{1 + (1 - \theta)\,Q(1 - \cos(\xi)) - i\,(1 - \theta)\sin(\xi)\lambda_1\gamma_\pm}\right\}.$$

As a consequence, the θ-scheme is stable if and only if

$$\frac{(1 - \theta Q(1 - \cos(\xi))^2 + \theta^2\sin^2(\xi)(\lambda_1\gamma_\pm)^2}{(1 + (1 - \theta)Q(1 - \cos(\xi)))^2 + (1 - \theta)^2\sin^2(\xi)(\lambda_1\gamma_\pm)^2} \le 1.$$

This condition is also written as

$$(2\theta-1)\sin^2(\xi)(\lambda_1\gamma_\pm)^2 \leq (2+(1-2\theta)Q(1-\cos(\xi)))Q(1-\cos(\xi)).$$

Since $|\gamma_+| \geq |\gamma_-|$, the θ-scheme is stable if

$$(2\theta-1)\sin^2(\xi)(\lambda_1\gamma_+)^2 \leq (2+(1-2\theta)Q(1-\cos(\xi)))Q(1-\cos(\xi)).$$

As a consequence, the θ-scheme is always stable if $\theta \leq 1/2$. Let us now consider the case $\theta > 1/2$: then one has the following CFL condition:

$$(2\theta-1)^2\lambda_1^2 \leq \frac{2-(2\theta-1)Q(1-\cos(\xi)(2\theta-1)Q(1-\cos(\xi))}{(1+\cos(\xi))(|\bar{u}|+\sqrt{\bar{c}^2+2\frac{\bar{\sigma}\lambda_3}{\lambda_1}(1-\cos(\xi))})^2},$$

The discussion is now similar to the one carried out in the explicit case $\theta = 0$, namely

$$(2\theta-1)^2\lambda_1^2 \leq R\left(Q(2\theta-1), \frac{\lambda_3}{\lambda_1}, |u|, c\right).$$

This conclude the proof of the proposition. □

Remark 2.9. *Note that for the Crank Nicolson scheme, $\theta = 1/2$, one can choose $Q = 0$ a classical centered scheme. In this case, this corresponds to the numerical schemes used for the practical simulation of thin film flows down an inclined plane in the presence of surface tension [KRSV].*

2.2.2 Second order accurate schemes

Hereafter, we consider second order accurate schemes and consider Lax-Friedrichs fluxes . For the time discretization, we consider the Runge Kutta (second order accurate) method and the Crank Nicolson method. Assume that the linearized Euler-Korteweg equations are written as

$$v_t + A\partial_x v = B\partial_{xxx}v.$$

We discretize in space by using a MUSCL scheme [Col, VL] for the first order differential operator without nonlinear monotony correction of the slope (it does not operate in the smooth monotone area of the solution), and centered approximation of third order differential terms :

$$\frac{dv_j}{dt} = -\frac{\triangle_+ g_{LF}\left(v_{j-1/2,-}, v_{j-1/2,+}\right)}{\delta x} + \frac{B}{2\delta x^3}\left(v_{j+2}-2v_{j+1}+2v_{j-1}-v_{j-2}\right)$$

where $v_{j-1/2,-} = v_{j-1} + \frac{d_{j-1}}{2}$, $v_{j-1/2,+} = v_j - \frac{d_j}{2}$, d_j is the local increment of v given (without monotonicity correction) by the centered formula $d_j = \frac{v_{j+1}-v_{j-1}}{2}$:

$$\frac{dv_j}{dt} = \frac{A\left(v_{j+2} - 6v_{j+1} + 6v_{j-1} - v_{j-2}\right)}{8\delta x} + \frac{Q}{2\lambda_1}\frac{\left(-v_{j+2} + 4v_{j+1} - 6v_j + 4v_{j-1} - v_{j-2}\right)}{8\delta x} + \frac{B}{2\delta x^3}\left(v_{j+2} - 2v_{j+1} + 2v_{j-1} - v_{j-2}\right) \tag{2.10}$$

with $j \in \mathbb{Z}$. We search for solutions of (2.10) in the form $v_j(t) = e^{-ij\xi}\hat{v}(t)$, one finds

$$\delta t\frac{d\hat{v}}{dt} = \mathcal{M}(\xi, Q, \lambda_1, \lambda_3)\hat{v}.$$

with

$$M_0(\xi, \lambda_1, \lambda_3) = \frac{\lambda_1}{2}A\left(3 - \cos(\xi)\right) + 2\lambda_3 B\left(1 - \cos(\xi)\right)$$

and

$$\mathcal{M}(\xi, Q, \lambda_1, \lambda_3) = -\frac{Q}{2}(1 - \cos(\xi))^2 Id + i\sin(\xi)M_0(\xi, \lambda_1, \lambda_3).$$

Then, the second order accurate scheme with explicit Runge-Kutta time discretization is written as

$$\hat{v}^{n+1} = \left(\mathrm{Id} + \mathcal{M}(\xi, Q, \lambda_1, \lambda_3) + \frac{1}{2}\mathcal{M}(\xi, Q, \lambda_1, \lambda_3)^2\right)\hat{v}^n,$$

The eigenvalues of $\mathcal{M}(\xi, Q, \lambda_1, \lambda_3)$ are given by $\lambda_\pm = -\frac{Q}{2}(1 - \cos(\xi))^2 - i\lambda_1\sin(\xi)\gamma_\pm$ with

$$\gamma_\pm = \frac{3 - \cos(\xi)}{2}\left(\bar{u} \pm \sqrt{\bar{c}^2 + \frac{4\bar{\sigma}\lambda_3(1 - \cos(\xi))}{\lambda_1(3 - \cos(\xi))}}\right)$$

In order to simplify notations, we introduce $\tilde{Q} = \frac{Q}{2}(1-\cos(\xi))^2$ and $\Lambda_1 = \lambda_1\gamma_\pm\sin(\xi)$. Then, the second order accurate scheme with Runge Kutta time discretization is stable if and only if

$$\left|(1 - \tilde{Q} - i\Lambda_1 + \frac{\left(-\tilde{Q} - i\Lambda_1\right)^2}{2}\right|^2 \leq 1$$

or equivalently

$$\frac{\Lambda_1^2}{2} \leq \tilde{Q} - \frac{\tilde{Q}^2}{2} + \sqrt{2\tilde{Q} - \tilde{Q}^2}$$

With $\tilde{Q} = \frac{1}{2}Qx$ and $\Lambda_1^2 = \lambda_1^2 x\,(2-x)\left(\frac{2+x}{2}\right)^2\left(\bar{u}+\sqrt{\bar{c}^2+\frac{4\bar{\sigma}\lambda_3 x}{\lambda_1(2+x)}}\right)^2$.

As a result, the explicit second order accurate scheme (MUSCL) is stable only if

$$\lambda_1^2\left(\bar{u}+\sqrt{\bar{c}^2+\frac{4\bar{\sigma}x}{\delta x^2\,(2+x)}}\right)^2 \leq 4\frac{\sqrt{4Q-Q^2x^2}+Qx-\frac{Q^2x^3}{4}}{(2-x)(2+x)^2}$$

and we have proved the following proposition.

Proposition 2.10. *The second order accurate scheme with MUSCL type discretization in space and Runge Kutta time discretization is stable if and only if* $0 < Q \leq 1$ *and*

$$\lambda_1^2\left(\bar{u}+\sqrt{\bar{c}^2+\frac{4\bar{\sigma}x}{\delta x^2\,(2+x)}}\right)^2 \leq 4\frac{\sqrt{4Q-Q^2x^2}+Qx-\frac{Q^2x^3}{4}}{(2-x)(2+x)^2}$$

for all $x \in [0,2]$.

Corollary 2.11. *The classical Lax-Friedrichs scheme with MUSCL space discretization is stable in the Von Neumann sense if*

$$\lambda_1\left(\bar{u}+\sqrt{\bar{c}^2+\frac{2\bar{\sigma}}{\delta x^2}}\right) \leq 1$$

When δx *is sufficiently small one finds the following condition, :*

$$\frac{\delta t}{\delta x^{\frac{7}{3}}} \leq \left(\frac{\sqrt{(\bar{u}+\bar{c})}}{\bar{\sigma}}\right)^{\frac{2}{3}}\frac{7^{\frac{7}{6}}\sqrt{3}}{24}+O\left(\delta x\right)+O\left(\sqrt{\lambda_1}\right)$$

for the Rusanov scheme with MUSCL space discretization

Remark 2.12. *For the classical Lax Friedrichs scheme, the CFL stability condition has the same nature than in the case of first order accurate schemes whereas we get an improved CFL condition for the Rusanov scheme in comparison to first order accurate schemes.*

We finish this section by checking the stability of an other second order scheme, namely the Crank Nicolson scheme (θ-scheme with $\theta = 1/2$). We prove the following proposition.

Proposition 2.13. *The difference approximation with Crank Nicolson time discretization and second order accurate in space (MUSCL with Lax-Friedrichs fluxes) is stable for all $Q \geq 0$.*

Proof. This Crank-Nicolson scheme for (2.10) reads

$$\hat{v}^{n+1} = \left(1 - \frac{1}{2}\mathcal{M}(\xi, Q, \lambda_1, \lambda_3)\right)^{-1} \left(1 + \frac{1}{2}\mathcal{M}(\xi, Q, \lambda_1, \lambda_3)\right) \hat{v}^n.$$

It is stable if and only if

$$\left| \frac{1 - \frac{Q}{4}(1-\cos(\xi))^2 + i\frac{\lambda_1}{2}\sin(\xi)\gamma_\pm}{1 + \frac{Q}{4}(1-\cos(\xi))^2 - i\frac{\lambda_1}{2}\sin(\xi)\gamma_\pm} \right| \leq 1$$

It is easily seen that this condition is equivalent to

$$(4 - Q(1-\cos(\xi))^2)^2 + (2\lambda_1\gamma_\pm)^2 \leq (4 + Q(1-\cos(\xi))^2)^2 + (2\lambda_1\gamma_\pm)^2,$$

which obviously holds true for any $Q \geq 0$, and concludes the proof of the proposition. □

3 Entropy stability of difference approximations

In this section, we study the entropy stability of difference approximations for Euler-Korteweg equations (1.1). Recall that (ρ, u) solution of (1.1) satisfies the energy estimate

$$\partial_t \int_{\mathbb{T}} \rho\frac{u^2}{2} + F(\rho) + \kappa(\rho)\frac{(\partial_x\rho)^2}{2} = 0,$$

with $\mathbb{T} = \mathbb{R}/L\mathbb{Z}$ for any $L > 0$. The surface tension plays a significant role in the energy estimate and the previous section illustrates that it is a non trivial task to obtain a numerical scheme which conserves or, at least, dissipates the energy, even at the linearized level.

In this section, we introduce a new unknown $w = \sqrt{\kappa(\rho)}\partial_x\rho/\sqrt{\rho}$ and derive an evolution equation for w. The system of evolution PDEs for $(\rho, \rho u, \rho w)$ is made of a first order hyperbolic part perturbed by a second order anti dissipative term. This latter term is discretized by centered finite differences. We show that any entropy dissipative schemes for the hyperbolic part (in the sense defined by Tadmor in [T]), provides an entropy dissipative scheme for the "augmented" Euler-Korteweg system. Then we consider fully discrete schemes and show that (FE) time discretization is entropy stable under a suitable CFL condition which is consistent with the one derived in the previous section whereas (BE) time discretization is always stable.

3.1 "Schrödinger" formulation of the Euler-Korteweg system

We start from the Euler-Korteweg system written in $(\rho, \rho u)$ variables: by setting $w = \sqrt{\kappa(\rho)}\partial_x\rho/\sqrt{\rho}$, one finds the augmented Euler Korteweg system

$$\partial_t\rho + \partial_x(\rho u) = 0, \tag{3.1}$$

$$\partial_t(\rho u) + \partial_x(\rho u^2 + P(\rho)) = \partial_x\left(\mu(\rho)\partial_x w\right), \tag{3.2}$$

$$\partial_t(\rho w) + \partial_x(\rho u\, w) = -\partial_x\left(\mu(\rho)\partial_x u\right), \tag{3.3}$$

with $\mu(\rho) = \rho^{3/2}\sqrt{\kappa(\rho)}$. The equation (3.3) is derived from the mass conservation law (3.1). In order to simplify notations, we introduce $v = (\rho, \rho u, \rho w)^T$ and $f(v) = (\rho u, \rho u^2 + P(\rho), \rho u w)^T$: then the system (3.1-3.3) reads

$$\partial_t v + \partial_x f(v) = \partial_x\left(B(\rho)\partial_x\, z\right), \tag{3.4}$$

where $z = \rho^{-1}v$ and $B(\rho)$ denotes the skew-symmetric matrix

$$B(\rho) = \begin{pmatrix} 0 & 0 & 0 \\ 0 & 0 & \mu(\rho) \\ 0 & -\mu(\rho) & 0 \end{pmatrix}.$$

Note that the first order part of (3.4) ($B(\rho) = 0$) admits an entropy-entropy flux pair (U, G) with

$$U(v) = F(\rho) + \rho\frac{u^2 + w^2}{2}, \quad G(v) = u\left(U(v) + P(\rho)\right)$$

whereas the augmented Euler-Korteweg system (3.4) admits an additional conservation law

$$\partial_t U(v) + \partial_x G(v) = \partial_x\left(\mu(\rho)(u\partial_x w - w\partial_x u)\right).$$

We consider difference approximations of (3.4) in the conservative form

$$\frac{d}{dt}v_j(t) + \frac{f_{j+\frac{1}{2}} - f_{j-\frac{1}{2}}}{\delta x} = \frac{1}{\delta x^2}\Big(B(\rho_{j+\frac{1}{2}})\left(z_{j+1} - z_j\right) - B(\rho_{j-\frac{1}{2}})\left(z_j - z_{j-1}\right)\Big). \tag{3.5}$$

Following the terminology used in [T], we enquire when the difference schemes (3.5) are *entropy stable* in the sense that there exists a numerical flux $\mathcal{G}_{j+\frac{1}{2}}$, which takes also into account the right hand side of (3.5), so that

$$\frac{d}{dt}U(v_j(t)) + \frac{\mathcal{G}_{j+\frac{1}{2}} - \mathcal{G}_{j-\frac{1}{2}}}{dx} \leq 0. \tag{3.6}$$

The difference approximation (3.5) is *entropy conservative* if the inequality in (3.6) is an equality. Note that any entropy-stable scheme satisfies the entropy inequality of the original system (1.1) in a weaker sense since $w_j(t)$ is an approximation of

$\sqrt{\kappa(\rho)}\partial_x\rho/\sqrt{\rho}$ at the point $x_j = j\,\delta x$. In the last section of the paper, we will use the Hamiltonian structure of (1.1) to obtain an entropy conservative scheme (for the semi discrete problem).

In what follows, we prove the following proposition.

Proposition 3.1. *Let us consider the finite difference scheme*

$$\frac{d}{dt}v_j(t) + \frac{f_{j+\frac{1}{2}} - f_{j-\frac{1}{2}}}{dx} = 0, \tag{3.7}$$

which is a semi discretization of (3.4) *with* $B = 0$ *and is entropy stable. Then the difference scheme* (3.5) *is entropy stable.*

Proof. The difference approximation (3.7) is entropy stable, then there exists a consistent entropy flux $\mathcal{F}_{j+\frac{1}{2}}$ so that

$$U_v(v_j)^T \frac{f_{j+\frac{1}{2}} - f_{j-\frac{1}{2}}}{\delta x} = \frac{\mathcal{F}_{j+\frac{1}{2}} - \mathcal{F}_{j-\frac{1}{2}}}{\delta x} + \mathcal{R}_j,$$

with $\mathcal{R}_j \geq 0$. Let us now consider the difference scheme (3.5) and multiply this equation by $U_v(v_j)^T$: one finds

$$\frac{d}{dt}U(v_j) + \frac{\mathcal{F}_{j+\frac{1}{2}} - \mathcal{F}_{j-\frac{1}{2}}}{\delta x} + \mathcal{R}_j = \underbrace{\frac{U_v(v_j)^T}{\delta x^2}\Big(B(\rho_{j+\frac{1}{2}})\big(z_{j+1} - z_j\big) - B(\rho_{j-\frac{1}{2}})\big(z_j - z_{j-1}\big)\Big)}_{:=\mathcal{K}_j},$$

We focus on the "capillary" term $\mathcal{K}_j$: it is written as

$$\begin{aligned} \delta x^2 \mathcal{K}_j &= u_j\left(\mu_{j+\frac{1}{2}}(w_{j+1} - w_j) - \mu_{j-\frac{1}{2}}(w_j - w_{j-1})\right) \\ &\quad - w_j\left(\mu_{j+\frac{1}{2}}(u_{j+1} - u_j) - \mu_{j-\frac{1}{2}}(u_j - u_{j-1})\right) \\ &= \mu_{j+\frac{1}{2}}\left(u_j w_{j+1} - u_{j+1}w_j\right) - \mu_{j-\frac{1}{2}}\left(u_{j-1}w_j - u_j w_{j-1}\right) \end{aligned} \tag{3.8}$$

Then, we introduce the entropy flux $\mathcal{G}_{j+\frac{1}{2}}$:

$$\mathcal{G}_{j+\frac{1}{2}} = \mathcal{F}_{j+\frac{1}{2}} - \mu_{j+\frac{1}{2}}\frac{u_j w_{j+1} - u_{j+1}w_j}{\delta x}.$$

This numerical entropy flux is clearly consistent with the continuous entropy flux of the augmented Euler Korteweg system

$$\mathcal{G}(\rho, u, w, \partial_x u, \partial_x w) = u\left(U(v) + P(\rho)\right) - \mu(\rho)\left(u\partial_x w - w\partial_x u\right),$$

provided the entropy flux $\mathcal{F}_{j+\frac{1}{2}}$ is consistent with the entropy flux $G(v)$ of the hyperbolic part of (3.1-3.3). Moreover, we have the following semi discrete entropy estimate

$$\frac{d}{dt}U(v_j) + \frac{\left(\mathcal{G}_{j+\frac{1}{2}} - \mathcal{G}_{j-\frac{1}{2}}\right)}{\delta x} = -\mathcal{R}_j \leq 0.$$

This completes the proof of the proposition. $\square$

By applying the proposition (3.1) and considering the analysis of various entropy stable schemes found in [T], one finds that many of the classical three points (first order) schemes (Rusanov scheme, Lax Friedrichs scheme, Harten-Lax-van Leer scheme) provide natural entropy stable schemes for the augmented Euler-Korteweg system ((3.1)-(3.3)). For application purposes, we check the entropy stability of *fully discrete schemes.*

3.2 Entropy stability of fully-discrete schemes

In this section, we restrict our discussion to the backward implicit and the forward explicit Euler time discretization which read, respectively:

$$\begin{aligned} & v_j^{n+1} - v_j^n + \lambda_1 \left(f_{j+\frac{1}{2}}^{n+1} - f_{j-\frac{1}{2}}^{n+1}\right) \\ & \qquad = \lambda_2 \left(B(\rho_{j+\frac{1}{2}}^{n+1})\left(z_{j+1}^{n+1} - z_j^{n+1}\right) - B(\rho_{j-\frac{1}{2}}^{n+1})\left(z_j^{n+1} - z_{j-1}^{n+1}\right)\right). \end{aligned} \tag{3.9}$$

$$\begin{aligned} & v_j^{n+1} - v_j^n + \lambda_1 \left(f_{j+\frac{1}{2}}^{n} - f_{j-\frac{1}{2}}^{n}\right) \\ & \qquad = \lambda_2 \left(B(\rho_{j+\frac{1}{2}}^{n})\left(z_{j+1}^{n} - z_j^{n}\right) - B(\rho_{j-\frac{1}{2}}^{n})\left(z_j^{n} - z_{j-1}^{n}\right)\right). \end{aligned} \tag{3.10}$$

We first prove the entropy stability of the implicit backward Euler time discretization.

Proposition 3.2. *Let us consider the semi discretized scheme*

$$\frac{d}{dt}v_j(t) + \frac{f_{j+\frac{1}{2}} - f_{j-\frac{1}{2}}}{dx} = 0, \tag{3.11}$$

which is an entropy stable approximation of (3.4) *with* $B = 0$*. Then the associated (BE) time discretization* (3.9) *is always entropy stable: there exists* $\mathcal{G}_{j+\frac{1}{2}}^n$ *so that*

$$U(v_j^{n+1}) - U(v_j^n) + \frac{\delta t}{\delta x}(\mathcal{G}_{j+\frac{1}{2}}^n - \mathcal{G}_{j-\frac{1}{2}}^n) \leq 0, \forall j, \quad \forall n. \tag{3.12}$$

Proof. The entropy U is a convex function of the variables $v = (\rho, u, w)$: then one has

$$U(v_j^{n+1}) \leq U(v_j^n) + U_v(v_j^{n+1})^T(v_j^{n+1} - v_j^n). \tag{3.13}$$

The semi-discrete scheme (3.11) is entropy stable so that

$$U_v(v_j^{n+1})^T(f_{j+\frac{1}{2}}^{n+1} - f_{j-\frac{1}{2}}^{n+1}) = \mathcal{F}_{j+\frac{1}{2}}^{n+1} - \mathcal{F}_{j-\frac{1}{2}}^{n+1} + \mathcal{R}_j^n,$$

with $\mathcal{R}_j^n \geq 0$. Moreover, one has

$$\begin{aligned} &U_v(v_j^{n+1})^T \Big(B(\rho_{j+\frac{1}{2}}^{n+1})\big((\rho^{-1}v)_{j+1}^{n+1} - (\rho^{-1}v)_j^{n+1}\big) - B(\rho_{j-\frac{1}{2}}^{n+1})\big((\rho^{-1}v)_j^{n+1} - (\rho^{-1}v)_{j-1}^{n+1}\big)\Big) \\ &\qquad = \mu_{j+\frac{1}{2}}^{n+1}\left(u_j^{n+1}w_{j+1}^{n+1} - u_{j+1}^{n+1}w_j^{n+1}\right) - \mu_{j-\frac{1}{2}}^{n+1}\left(u_{j-1}^{n+1}w_j^{n+1} - u_j^{n+1}w_{j-1}^{n+1}\right). \end{aligned} \tag{3.14}$$

Now we introduce the entropy flux $\mathcal{G}_{j+\frac{1}{2}}^n$:

$$\mathcal{G}_{j+\frac{1}{2}}^n = \mathcal{F}_{j+\frac{1}{2}}^{n+1} - \mu_{j+\frac{1}{2}}^{n+1}\frac{u_j^{n+1}w_{j+1}^{n+1} - u_{j+1}^{n+1}w_j^{n+1}}{\delta x}$$

Then, by inserting (3.9) into (3.13) and by using the definition of $\mathcal{G}_{j+\frac{1}{2}}^n$, one obtains

$$U(v_j^{n+1}) - U(v_j^n) + \lambda_1(\mathcal{G}_{j+\frac{1}{2}}^n - \mathcal{G}_{j-\frac{1}{2}}^n) \leq -\lambda_1\mathcal{R}_j^n \leq 0.$$

This completes the proof of the proposition. □

Next, we consider the entropy stability of the forward explicit Euler scheme (3.10). Hereafter, we focus on conservative schemes which admit the following viscosity form:

$$\frac{d}{dt}v_j + \frac{f(v_{j+1}) - f(v_{j-1})}{2\delta x} = \frac{1}{2\delta x}\Big(Q_{j+\frac{1}{2}}(\tilde{z}_{j+1} - \tilde{z}_j) - Q_{j-\frac{1}{2}}(\tilde{z}_j - \tilde{z}_{j-1})\Big), \tag{3.15}$$

so that the flux $f_{j+\frac{1}{2}}$ reads

$$f_{j+\frac{1}{2}} = \frac{f(v_{j+1}) + f(v_j)}{2} - \frac{1}{2}Q_{j+\frac{1}{2}}(\tilde{z}_{j+1} - \tilde{z}_j).$$

The matrix $Q_{j+\frac{1}{2}}$ is a symmetric matrix whereas $\tilde{z} = U_v(v)$ represent the entropy variables. It is easily seen that $\tilde{z}_2 = z_2 = u$ and $\tilde{z}_3 = z_3 = w$. Here the conservative variables v are considered as functions of the entropy variables: in particular $v_j = v(\tilde{z}_j)$. The classical Lax-Friedrichs scheme and Rusanov scheme are particular cases of (3.15). Indeed, these schemes have the particular form

$$\frac{d}{dt}v_j + \frac{f(v_{j+1}) - f(v_{j-1})}{2\delta x} = \frac{1}{2\delta x}\Big(p_{j+\frac{1}{2}}(v_{j+1} - v_j) - p_{j-\frac{1}{2}}(v_j - v_{j-1})\Big), \tag{3.16}$$

with $p_{j+\frac{1}{2}} \geq 0$ a numerical viscosity. Indeed, one has

$$\left(\int_0^1 v_{\tilde{z}}(\tilde{z}_j + \xi(\tilde{z}_{j+1} - \tilde{z}_j))d\xi\right)(\tilde{z}_{j+1} - \tilde{z}_j) = v_{j+1} - v_j$$

$$v_{\tilde{z}} = (\tilde{z}_v)^{-1} = (U_{vv})^{-1}$$

then $v_{\tilde{z}} = v_{\tilde{z}}^T$, so that (3.16) is a particular case of (3.15) by setting

$$Q_{j+\frac{1}{2}} = p_{j+\frac{1}{2}} \int_0^1 v_{\tilde{z}}(\tilde{z}_j + \xi(\tilde{z}_{j+1} - \tilde{z}_j))d\xi.$$

with $Q_{j+\frac{1}{2}} = Q^T_{j+\frac{1}{2}}$. Following [T], one can compare the conservative scheme (3.15) with the entropy conservative scheme through the relation:

$$\begin{aligned}\langle \tilde{z}_j, f_{j+\frac{1}{2}} - f_{j-\frac{1}{2}}\rangle =& \mathcal{F}_{j+\frac{1}{2}} - \mathcal{F}_{j-\frac{1}{2}} \\ &+ \frac{1}{4}\left(\langle(\tilde{z}_{j+1} - \tilde{z}_j), D_{j+\frac{1}{2}}(\tilde{z}_{j+1} - \tilde{z}_j)\rangle + \langle(\tilde{z}_j - \tilde{z}_{j-1}), D_{j-\frac{1}{2}}(\tilde{z}_j - \tilde{z}_{j-1})\rangle\right),\end{aligned} \tag{3.17}$$

with $D_{j+\frac{1}{2}} = Q_{j+\frac{1}{2}} - Q^*_{j+\frac{1}{2}}$ where $Q^*_{j+\frac{1}{2}}$ is the numerical viscosity matrix of the conservative scheme:

$$Q^*_{j+\frac{1}{2}} = \int_{-1/2}^{1/2} 2\xi C\left(\frac{\tilde{z}_{j+1} + \tilde{z}_j}{2} + \xi(\tilde{z}_{j+1} - \tilde{z}_j)\right)d\xi$$

with $C(z) = g_z(z)$ and $g(z) = f(v(z))$ whereas $\mathcal{F}_{j+\frac{1}{2}}$ is a consistent numerical entropy flux. We prove the following proposition.

Proposition 3.3. *The (FE) finite difference scheme:*

$$\begin{aligned}&v_j^{n+1} - v_j^n + \lambda_1(f_{j+\frac{1}{2}} - f_{j-\frac{1}{2}}) = \lambda_2\left(B^n_{j+\frac{1}{2}}(z^n_{j+1} - z^n_j) - B^n_{j-\frac{1}{2}}(z^n_j - z^n_{j-1})\right),\\ &f^n_{j+\frac{1}{2}} = \frac{f(v^n_{j+1}) + f(v^n_j)}{2} - \frac{1}{2}Q^n_{j+\frac{1}{2}}(z^n_{j+1} - z^n_j).\end{aligned} \tag{3.18}$$

is entropy stable, i.e. there exists a numerical entropy flux $\mathcal{G}^n_{j+\frac{1}{2}}$ so that

$$U(v_j^{n+1}) - U(v_j^n) + \lambda_1(\mathcal{G}^n_{j+\frac{1}{2}} - \mathcal{G}^n_{j-\frac{1}{2}}) \leq 0,$$

under the following CFL condition

$$M_j^n\left(\lambda_1 N^n_{j+\frac{1}{2}} + \lambda_2\|B^n_{j+\frac{1}{2}}\|\right)^2 \leq \lambda_1 \min(\mathrm{Sp}(D^n_{j+\frac{1}{2}})),$$

with $M_j^n, N_{j+\frac{1}{2}}^n$ *defined as*

$$M_j^n = \sup_{\xi\in(0,1)} \|U_{vv}(v_j^n + .(v_j^{n+1} - v_j^n))\|,$$
$$N_{j+\frac{1}{2}}^n = \int_0^1 \|C\left(\tilde{z}_j^n + \xi(\tilde{z}_{j+1}^n - \tilde{z}_j^n)\right)\|d\xi + \|Q_{j+\frac{1}{2}}^n\|.$$

Proof. We first apply the Taylor Lagrange formula to U:

$$U(v_j^{n+1}) = U(v_j^n) + U_v(v_j^n)^T(v_j^{n+1} - v_j^n) + \int_0^1 (1-\xi)(v_j^{n+1} - v_j^n)^T U_{vv}(v_j^n + \xi(v_j^{n+1} - v_j^n))(v_j^{n+1} - v_j^n)d\xi.$$

Then, by using (3.17), one finds

$$\begin{aligned} U(v_j^{n+1}) - U(v_j^n) + \lambda_1\left(\mathcal{F}_{j+\frac{1}{2}}^n - \mathcal{F}_{j-\frac{1}{2}}^n\right) &= \int_0^1 (1-\xi)(v_j^{n+1} - v_j^n)^T U_{vv}(v_j^n + \xi(v_j^{n+1} - v_j^n))(v_j^{n+1} - v_j^n)d\xi \\ &\quad - \frac{\lambda_1}{4}\left((\tilde{z}_{j+1}^n - \tilde{z}_j^n)^T D_{j+\frac{1}{2}}^n(\tilde{z}_{j+1}^n - \tilde{z}_j^n) + (\tilde{z}_j^n - \tilde{z}_{j-1}^n)^T D_{j-\frac{1}{2}}^n(\tilde{z}_j^n - \tilde{z}_{j-1}^n)\right). \end{aligned} \tag{3.19}$$

The first term in the right hand side of (3.19) is positive and corresponds to entropy production due to the forward explicit Euler time discretization whereas the second term corresponds to entropy dissipation due to the spatial discretization. Next, we estimate the entropy production: in order to simplify notations, we set

$$\mathcal{I}_j^n = \int_0^1 (1-\xi)(v_j^{n+1} - v_j^n)^T U_{vv}(v_j^n + \xi(v_j^{n+1} - v_j^n))(v_j^{n+1} - v_j^n)d\xi.$$

One has

$$\mathcal{I}_j^n \le \frac{1}{2}\sup_{\xi\in(0,1)} \|U_{vv}(v_j^n + .(v_j^{n+1} - v_j^n))\|\|v_j^{n+1} - v_j^n\|^2 := \frac{1}{2}M_j^n\|v_{j+1}^n - v_j^n\|^2.$$

Next, we estimate $\|v_j^{n+1} - v_j^n\|$ by using (3.18): one finds

$$\|v_j^{n+1} - v_j^n\| \le \lambda_1\|f_{j+\frac{1}{2}}^n - f_{j-\frac{1}{2}}^n\| + \lambda_2\left(\|B_{j+\frac{1}{2}}^n\|\,\|z_{j+1}^n - z_j^n\| + \|B_{j-\frac{1}{2}}^n\|\|z_j^n - z_{j-1}^n\|\right).$$

On the other hand, one has

$$\begin{aligned} f_{j+\frac{1}{2}}^n - f_{j-\frac{1}{2}}^n &= \left(\int_0^1 C\left(\tilde{z}_j^n + \xi(\tilde{z}_{j+1}^n - \tilde{z}_j^n)\right)d\xi - Q_{j+\frac{1}{2}}^n\right)(\tilde{z}_{j+1}^n - \tilde{z}_j^n) \\ &\quad + \left(\int_0^1 C\left(\tilde{z}_j^n + \xi(\tilde{z}_j^n - \tilde{z}_{j-1}^n)\right)d\xi + Q_{j-\frac{1}{2}}^n\right)(\tilde{z}_j^n - \tilde{z}_{j-1}^n). \end{aligned}$$

Then, by setting $N^n_{j+\frac{1}{2}} = \int_0^1 \|C\left(\tilde{z}^n_j + \xi(\tilde{z}^n_{j+1} - \tilde{z}^n_j)\right)\|d\xi + \|Q^n_{j+\frac{1}{2}}\|$, one obtains

$$\|f^n_{j+\frac{1}{2}} - f^n_{j-\frac{1}{2}}\| \le N^n_{j+\frac{1}{2}}\|\tilde{z}^n_{j+1} - \tilde{z}^n_j\| + N^n_{j-\frac{1}{2}}\|\tilde{z}^n_j - \tilde{z}^n_{j-1}\|.$$

As a result, one finds that

$$\begin{aligned}\mathcal{I}^n_j &\le M^n_j\left(\lambda_1 N^n_{j+\frac{1}{2}} + \lambda_2\|B^n_{j+\frac{1}{2}}\|\right)^2\|\tilde{z}^n_{j+1} - \tilde{z}^n_j\|^2\\ &+ M^n_j\left(\lambda_1 N^n_{j-\frac{1}{2}} + \lambda_2\|B^n_{j-\frac{1}{2}}\|\right)^2\|\tilde{z}^n_j - \tilde{z}^n_{j-1}\|^2.\end{aligned} \tag{3.20}$$

Next, we set $\Gamma^n_{j+\frac{1}{2}} = \min\left(\mathrm{Sp}(D^n_{j+1})\right)$. Furthermore, we assume that

$$M^n_j(\lambda_1 N^n_{j+\frac{1}{2}} + \lambda_2\|B^n_{j+\frac{1}{2}}\|)^2 \le \lambda_1\Gamma^n_{j+\frac{1}{2}}. \tag{3.21}$$

Then, by using (3.21) together with (3.20) and (3.19), one obtains entropy stability for the explicit forward Euler time discretization

$$U(v^{n+1}_j) - U(v^n_j) + \lambda_1(\mathcal{F}^n_{j+\frac{1}{2}} - \mathcal{F}^n_{j-\frac{1}{2}}) \le 0.$$

This completes the proof of the proposition. □

Let us consider Lax-Friedrichs schemes: by applying proposition 3.3, we prove the

Corollary 3.4. *Assume*

- *there exists* $K > 0$ *so that* $K^{-1} \le M^n_j \le K$ *for all* j, n,
- $p^n_{j+\frac{1}{2}} = \tilde{p}^n_{j+\frac{1}{2}} + \max\left(|\mathrm{Sp}(f_v(v^n_{j+1}))|, |\mathrm{Sp}(f_v(v^n_j))|\right)$.

The Lax Friedrichs type scheme, $\tilde{p}^n_{j+\frac{1}{2}} = \dfrac{\delta x}{2\delta t}$, *is entropy stable under the CFL condition*

$$K(\lambda_1 M_1(K) + \lambda_2 M_2(K))^2 \le \frac{1}{2},$$

for some constants $M_j(K), j = 1, 2$. *The Rusanov type scheme,* $\tilde{p}^n_{j+\frac{1}{2}} = \rho > 0$, *is entropy stable under the CFL condition*

$$K(\lambda_1 M_1(K) + \lambda_2 M_2(K))^2 \le \rho\lambda_1,$$

Remark 3.5. *The previous result states that the classical Lax-Friedrichs scheme is entropy stable if* $\delta t = O(\delta x^2)$ *whereas the Rusanov scheme is entropy stable only if* $\delta t = O(\delta x^3)$ *which is the Von Neumann stability criterion found in section 2.*

4 Numerical Simulations

4.1 Entropy stability: original vs new formulation

Before carrying out a numerical simulation of a Liu-Gollub experiment with the full shallow water system (1.2), we have considered the more simple situation of a fluid over an horizontal plane without friction at the bottom. The shallow water system reads

$$\partial_t h + \partial_x(hu) = 0, \quad \partial_t(hu) + \partial_x(hu^2 + g\frac{h^2}{2}) = \kappa h \partial_{xxx} h, \tag{4.1}$$

where $g = 9.8m.s^{-2}$ and $\kappa = \sigma/\rho$. The fluid under consideration in [LG] is an aqueous solution of glycerin with density $\rho = 1.134\,g.cm^{-3}$ and capillarity $\sigma = 67\,dyn.cm^{-1}$. The augmented form of (4.1) reads

$$\begin{aligned} &\partial_t h + \partial_x(hu) = 0, \\ &\partial_t(hu) + \partial_x(hu^2 + g\frac{h^2}{2}) = \sqrt{\kappa}\partial_x(h^{3/2}\partial_x w), \\ &\partial_t(hw) + \partial_x(huw) = -\sqrt{\kappa}\partial_x(h^{3/2}\partial_x u). \end{aligned} \tag{4.2}$$

We first tested the entropy stability of (second order accurate) difference approximations for the shallow water equations (4.1) and for its "Schrodinger type" counterpart (4.2). We work on a finite interval of length $X = 80cm$ with periodic boundary conditions. At time $t = 0$, the fluid velocity $u = 0$ and the fluid height is given by $h|_{t=0} = h_N\left(1 + 0.3\exp(-2000(x-0.4)^2)\right)$ with $h_N = 1mm$ (the characteristic fluid height in Liu-Gollub experiments). In order to capture correctly the capillary ripples, we have chosen $\delta x = 0.25mm$ and $\delta t = 120\delta x^2$. In figure 1, we draw the profile of the surface of the fluid at time $T = 1s$: as expected, the Lax-Friedrichs scheme slightly damps the capillary ripples in front of the shocks.

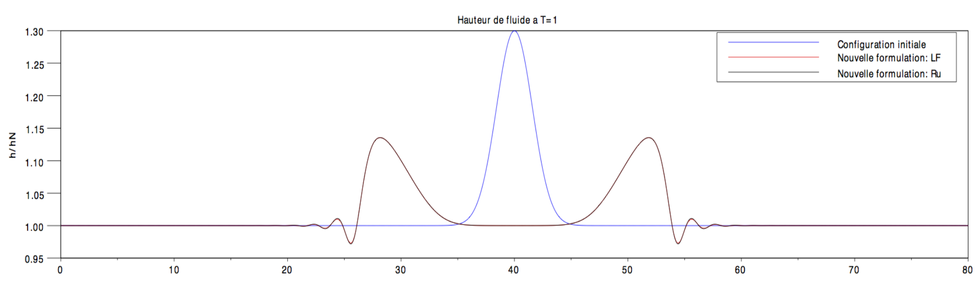

Figure 1: Profile of the surface of the fluid at time $T = 1$

In figure 2, we have drawn the relative entropy $\frac{U}{U|_{t=0}}$ as a function of time: the picture clearly indicates that the difference approximation of (4.2) have better entropy stability properties than difference approximation of (4.1).

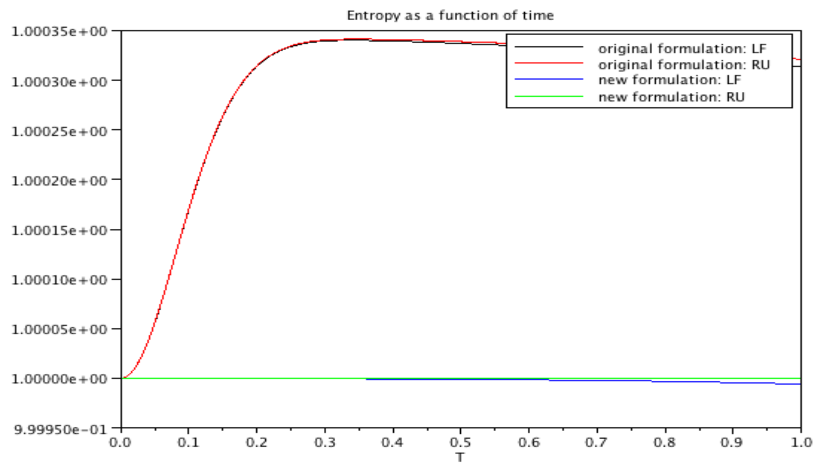

Figure 2: Entropy as a function of time: Comparison of the various spatial discretizations for the new formulation of (4.1). As expected, the entropy is almost constant for the difference approximations of (4.2). The results for the Harten-Lax-van Leer scheme are not plotted as the results are the same than the ones for the Rusanov scheme

A natural question arises about the new formulation: indeed one may ask whether the relation $hw = \frac{2}{3}\sqrt{\kappa}\partial_x(h^{3/2})$ is satisfied for all time. If not, it does not make sense to compare the performance with respect to entropy stability since it would represent two distinct quantities. In figure 3, we draw the relative error at time $T = 1$ and defined as

$$err_j = \frac{|(hw)_j - \sqrt{\kappa}\frac{h_{j+1}^{3/2} - h_{j-1}^{3/2}}{3\delta x}|}{\|hw\|}, \quad j = 1, \dots, N.$$

The numerical simulations show very good agreement, especially for the less dissipative schemes, Rusanov and Harten-Lax-van Leer, than for Lax-Friedrichs scheme. Moreover, it is easily seen that at the linearized level, the difference approximations of (4.2) and of (4.1) have comparable CFL conditions: in particular the CFL condition for Rusanov scheme is of the form $\delta t = O(\delta x^{7/3})$ that is rather close to the "optimal" heuristic CFL condition $\delta t = O(\delta x^2)$. Therefore, we can conclude from these numerical simulations that a difference approximation of (4.2) with a Rusanov flux

and second order accurate both in time and space is a natural candidate to perform numerical simulations of Liu-Gollub experiments [LG].

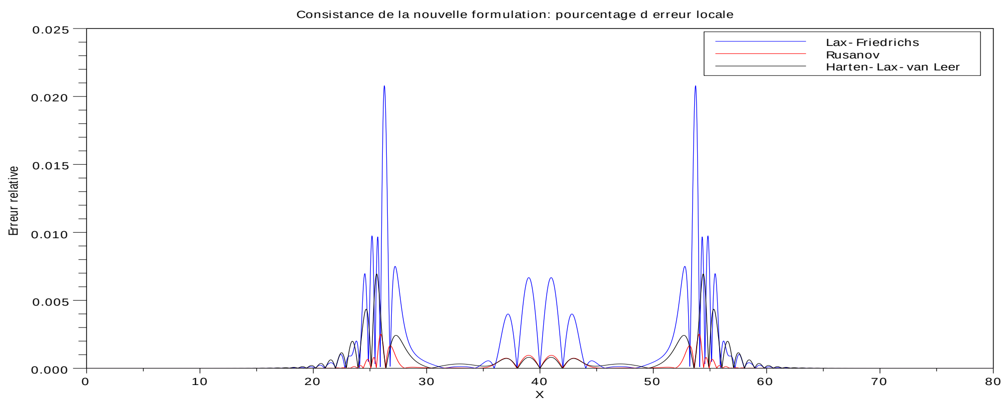

Figure 3: Consistency of the new formulation: relative error between the new variable hw and $\frac{2}{3}\sqrt{\kappa}\partial_x(h^{3/2})$. The Rusanov scheme and the Harten-Lax-Van Leer scheme have comparable consistency properties. In regards, the Lax Friedrichs scheme is less efficient to preserve consistency

4.2 A semi-discrete entropy conservative scheme

In this section, we use the Hamiltonian structure of the Euler-Korteweg equations to construct an entropy conservative scheme. For that purpose, we will write a semi discretized form of the Euler Korteweg system which respects its Hamiltonian structure so that the entropy conservation is automatically satisfied.

4.2.1 Derivation of a Hamiltonian difference approximation

We consider the Euler-Korteweg equations with periodic boundary conditions and, for $(\varrho, \mathrm{u}) = (\rho_i, u_i)_{i=1,\cdots,N}$, we introduce the discrete Hamiltonian

$$\mathrm{H}(\varrho, \mathrm{u}) = \sum_{i=1}^{N} \rho_i \frac{u_i^2}{2} + F(\rho_i) + \frac{1}{2}\kappa(\rho_i)\left(\frac{\rho_{i+1} - \rho_i}{\delta x}\right)^2. \tag{4.3}$$

We also introduce the symmetric matrix J

$$J = \begin{pmatrix} 0 & -\mathrm{I}_N \\ -\mathrm{I}_N & 0 \end{pmatrix},$$

and the difference operator D, defined in the space of N-periodic sequences in $\mathbb{R}^N$ as $Du_i = \frac{u_{i+1}-u_{i-1}}{2\delta x}$ (the associated matrix $D \in M_N(\mathbb{R})$ is skew symmetric). Then, we introduce the Hamiltonian system

$$\frac{d}{dt}\begin{pmatrix} \varrho \\ \mathrm{u} \end{pmatrix} = J \begin{pmatrix} D\nabla_\varrho \mathrm{H}(\varrho,\mathrm{u}) \\ D\nabla_\mathrm{u} \mathrm{H}(\varrho,\mathrm{u}) \end{pmatrix}. \tag{4.4}$$

More precisely, the discrete Hamiltonian system reads

$$\begin{aligned}
&\frac{d\rho_j}{dt} + \frac{(\rho u)_{j+1} - (\rho u)_{j-1}}{2\delta x} = 0,\\
&\frac{du_j}{dt} + \frac{u_{j+1}^2 - u_{j-1}^2}{4\delta x} + \frac{F'(\rho_{j+1}) - F'(\rho_{j-1})}{2\delta x}\\
&\qquad + \frac{1}{2\delta x}\left(\frac{\kappa'(\rho_{j+1})}{2}\left(\frac{\rho_{j+2}-\rho_{j+1}}{\delta x}\right)^2 - \frac{\kappa'(\rho_{j-1})}{2}\left(\frac{\rho_j - \rho_{j-1}}{\delta x}\right)^2\right)\\
&\qquad - \frac{1}{2\delta x^2}\left(\kappa(\rho_{j+1})\frac{\rho_{j+2}-\rho_{j+1}}{\delta x} - \kappa(\rho_j)\frac{\rho_{j+1}-\rho_j}{\delta x}\right)\\
&\qquad + \frac{1}{2\delta x^2}\left(\kappa(\rho_{j-1})\frac{\rho_j-\rho_{j-1}}{\delta x} - \kappa(\rho_{j-2})\frac{\rho_{j-1}-\rho_{j-2}}{\delta x}\right) = 0.
\end{aligned}$$

By construction, one has

$$\begin{aligned}
\frac{d}{dt}\mathrm{H}(\varrho,\mathrm{u}) &= \nabla_\varrho \mathrm{H}(\varrho,\mathrm{u})^T \frac{d\varrho}{dt} + \nabla_\mathrm{u} \mathrm{H}(\varrho,\mathrm{u})^T \frac{d\mathrm{u}}{dt}\\
&= \nabla_\varrho \mathrm{H}(\varrho,\mathrm{u})^T D\,\nabla_\mathrm{u}\mathrm{H}(\varrho,\mathrm{u}) + \nabla_\mathrm{u}\mathrm{H}(\varrho,\mathrm{u})^T D\,\nabla_\varrho \mathrm{H}(\varrho,\mathrm{u})\\
&= \nabla_\varrho \mathrm{H}(\varrho,\mathrm{u})^T (D + D^T)\,\nabla_\mathrm{u}\mathrm{H}(\varrho,\mathrm{u}) = 0.
\end{aligned}$$

It is clearly a consistent and first order discretization of the original system (1.3). At this stage, one can go one step further and derived naturally higher order entropy conservative scheme like in [CL]. Indeed, one easily improves the order of accuracy of (4.4) by considering a higher order approximation of the Hamiltonian and a higher order difference operator.

As a consequence, one is left with the problem of finding a time discretization that preserves the Hamiltonian structure. It is easily seen that an explicit forward Euler time integration is unstable whereas the backward implicit Euler time integration is entropy stable. In the linearized case, the Crank Nicolson scheme preserves exactly the Hamiltonian. The hamiltonian difference scheme derived here is based on centered difference and it is well known that for hyperbolic conservation laws, this could be a

source of numerical instabilities or spurious oscillatory modes. Though, the scheme considered here also provide a control on the gradient of the density and thus on oscillatory modes in addition of being more stable.

4.2.2 Numerical tests and dispersive shock waves

In what follows, we have tested the difference hamiltonian approximation of (4.1). In order to be entropy stable it is necessary to employ an implicit method: we have used here an implicit backward Euler time discretization. Due to the nonlinearity of the problem, the Crank-Nicolson, second order accurate, time discretization does not guarantee entropy stability. Therefore, we did not try to compare with other schemes tested in the previous section. An important remark is that now there is no numerical viscosity: a drawback is that the dynamical behavior is dramatically changed as shown in figure 4 and 5)

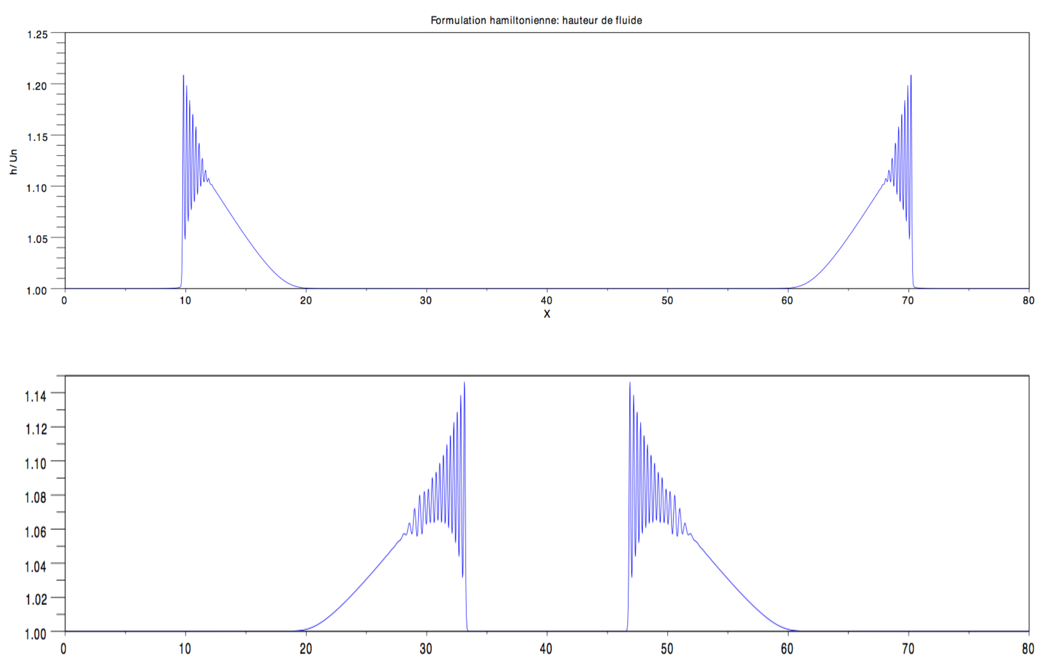

Figure 4: On top: Fluid height profile at time $T = 0.26$: after the breaking of the wave, an oscillatory part appears, due to dispersive regularization. On below: Fluid height profile at time T=0.66: the oscillatory zone is wider, characteristic of a dispersive shock wave

In order to see whether it is a numerical artifact, we checked the entropy stability of the difference hamiltonian approximation: the entropy remains clearly bounded with

time. Indeed, these oscillations are not a numerical artifact and can be explained (formally) by the theory of dispersive shock waves. Here, the classical hyperbolic shocks are smoothed by disperses effects: the oscillatory zone grows up in time and the oscillations are described by the Whitham modulations equations. This picture is not valid anymore in the presence of a slight amount of viscosity: there are still some oscillations but the width of the oscillatory zone stops growing after some time: see [J] and [EGK] for a detailed analysis respectively in the case of the Korteweg de Vries-Burgers equation and in the case of the Kaup system perturbed by a viscous term. In the previous section, a similar situation arises: the oscillatory zone stops growing as it is shown in the former computations in picture 1. Here the physical viscosity is replaced by numerical viscosity.

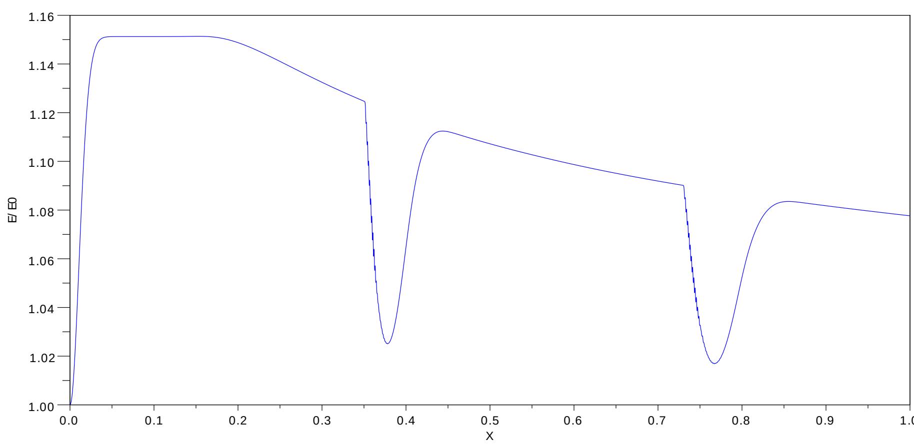

Figure 5: Entropy as a function of time. The behavior is rather similar to difference approximations in original variables: the entropy first increases then decreases with time: the “holes” in the decreasing part of the curve correspond to times when the bumps interact

4.3 Simulation of a Liu-Gollub experiment

In this section, we show a numerical simulation for a shallow water model derived for thin film flows down an inclined plane. The model lies in the family of first order

models derived in [NV]: it is written as
(4.5)

$$\partial_t h + \partial_x(hu) = 0,$$
$$\partial_t(hu) + \partial_x\left(hu^2 + P(h, A_1)\right) = A_1\left(gh\sin(\theta) - 3\frac{\nu u}{h} + \frac{\sigma}{\rho}h\partial_{xxx}h\right) + 4\nu\partial_{xx}q,$$

where $A_1 > 0$ and $P(h, A_1)$ is a pressure term given by

$$P(h, A_1) = A_1 g\cos(\theta)\frac{h^2}{2} + (\frac{4}{45} - \frac{2A_1}{25})\left(\frac{g\sin\theta}{\nu}\right)h^5.$$

Note that the viscous term $4\nu\partial_{xx}q$ is only heuristic so that the model is not a second order accurate model (with respect to the aspect ratio $\varepsilon = H/\lambda \ll 1$, $H \approx 1mm, \lambda \approx 1cm$). Here, the viscosity plays a significant role, $\nu = 6.28\,cS$. Indeed, the Reynolds number for this experiment is rather low: $Re = 29$ whereas the slope of the bottom is set to $\theta = 6.4^o$. The frequency of the perturbation at the inlet is $f = 1.5Hz$. We have chosen to carry out the numerical simulations with $A_1 = 1$. Following the conclusions of our study, we have chosed to carry out numerical simulations with a fully second order accurate scheme of the extended formulation of (4.5) and used a Rusanov flux for the first order part. Our numerical results show a good agreement with the experiment by Liu and Gollub [LG].
Up to now, the choice of boundary conditions for the Euler-Korteweg equations on a finite interval is an open problem so that we have chosed rather arbitrary boundary conditions. Furthermore, since the difference scheme contains numerical/physical viscosity, we have considered a set of 5 boundary conditions. First, at the inlet, we chosed:

$$h|_{x=0} = h_N\left(1 + 0.03\sin(2\pi\, f\, t)\right), \quad q|_{x=0} = q_N, \quad \partial_x h|_{x=0} = 0.$$

In contrast to [KRSV], we have chosed free boundary conditions at the outlet:

$$\partial_x h|_{x=L} = \partial_x q|_{x=L} = 0$$

instead of "hyperbolic type" boundary conditions where h and q are advected with an artificial velocity $V_{out} > 0$. As pointed out in [KRSV] the choice of the boundary conditions at the outlet does not seem to influence the dynamic within the channel (no reflection waves).

5 Concluding remarks

In this paper, we considered the stability of various difference approximations of the Euler-Korteweg equations with applications to shallow water equations with surface

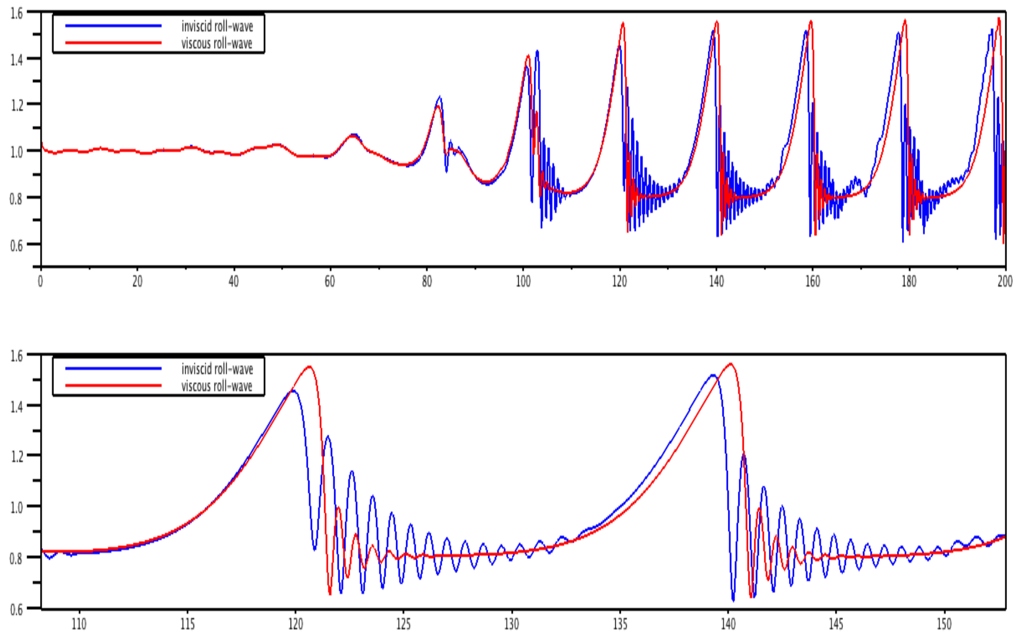

Figure 6: Simulation of Liu Gollub experiment [LG]: the Reynolds number is $Re = 29$ and the inclination is $\theta = 6.4^o$. The frequency at the inlet if $f = 1.5Hz$. On top: a picture of the complete experiment, from the inlet to the outlet (2m). On below: a zoom over one spatial period when roll-wave profiles are stabilized

tension. A first class of difference approximations is built by considering the Euler-Korteweg system as the classic isentropic compressible Euler equations perturbed by a disperse term. This latter term is discretized with centered finite differences and various classical scheme for the convection part are considered. It is proved that a certain amount of numerical viscosity is needed to obtain difference schemes that are stable in the von Neumann sense (under suitable CFL conditions).

In order to get entropy stability, we considered an extended formulation of the Euler Korteweg equations and proved entropy stability of Lax-Friedrichs type schemes. We have shown numerically that the extended formulation of the Euler-Korteweg system has better stability properties than the original one. We also carry out a numerical simulation of a shallow water system which models an experiment by Liu and Gollub to observe roll-waves [LG].

By considering the Euler-Korteweg system as a Hamiltonian system of evolution PDEs, we introduced a semi-discretized difference approximations which preserves the Hamiltonian structure. This scheme has no numerical viscosity so that it is particularly useful to study purely dispersive Euler Korteweg system: in particular,

one can find numerically the dispersive shock waves [E] of the Euler-Korteweg system.

Several questions remain open. First, we carried out a numerical simulation of the Liu Gollub experiment by choosing rather arbitrary boundary conditions. In fact, the choice of suitable boundary conditions for the Euler Korteweg system on a finite interval in order to prove well posedness is still an open problem. A first attempt in this direction is found in [A] where the well posedness of the linearized Euler-Korteweg equations is proved on a half space under a generalized Lopatinskii condition.

Furthermore, we restricted our attention to one dimensional problem. For thin film flows, this restricts the study to primary instabilities: in order to analyze secondary instabilities found experimentally [LSG], one has consider $2d$ problems. In that setting, an extended formulation is still available [BDDd] so that we expect our analysis extends easily, at least to cartesian meshes. An other interesting question is the extension of this analysis to other mixed hyperbolic/dispersive equations like the Boussinesq equations or the Serre/Green-Naghdi equations. Up to now, the strategy adopted to deal with these system is time splitting without proof of stability (though numerical results are rather satisfying).

Finally an other open interesting question concerns the time integration of the hamiltonian semi-discrete approximation: here, we have used a backward implicit Euler time integration so as to be entropy stable but it does not preserve the hamiltonanian (nor a perturbation of it). This kind of method are particularly of interest in order to study the nonlinear stability of various traveling waves solutions of the purely dispersive equations.

References

[A] C. Audiard *Non homogeneous boundary value problems for linear dispersive equations*, Comm. Parti. Diff. Eqs 37 (2012) no 1, p. 1-37

[BDD] S. Benzoni-Gavage, R. Danchin, S. Descombes *Well-posedness of one-dimensional Korteweg models*, Electronic J. Diff. Equations 59 (2006), pp. 1-35.

[BDDd] S. Benzoni-Gavage, R. Danchin, S. Descombes *On the well-posedness for the Euler-Korteweg model in several space dimensions*, Indiana Univ Math Journal 56 (2007), no 4, pp. 1499-1579.

[CL] C. Chalons, P.G. LeFloch *High-Order Entropy-Conservative Scheme and Kinetic Relations for Van der Waals Fluids*, Journal of Computational Physics 168 (2001) 184-206.

[Col] F. Coquel, P.G. LeFloch *An entropy satisfying MUSCL scheme for systems of conservation laws* Numer. Math. 74 (1996) 1-33.

[E] G. A. El, *Resolution of a shock in hyperbolic systems modified by weak dispersion* Chaos, 15 (3): 037103, 21, 2005.

[EGK] G. A. El, R. H. J. Grimshaw, and A.M. Kamchatnov, *Analytic model for a weakly dissipative shallow water undular bore* Chaos, 15 (3): 037102, 2005.

[EGS] G. A. El, R. H. J. Grimshaw, and N. F. Smyth. *Unsteady undular bores in fully nonlinear shallow-water theory.* Physics of Fluids, 18(2):027104, February 2006.

[J] S. Johnson *A non-linear equation incorporating damping and dispersion* J. Fluid. Mech. 42 (1970) p. 49-60.

[KRSV] S. Kalliadasis, C. Ruyer-Quil, B. Scheid, M.G. Velarde *Falling Liquid Films*, Applied Mathematical Sciences 176 (2012)

[LMR] P.G. LeFloch, J.M. Mercier, C. Rohde *Fully discrete, entropy conservative schemes of arbitrary order*, SIAM J. Numer. Anal. 40 (2002) No 5, pp 1968-1992.

[LG] J. Liu, J.P. Gollub *Solitary wave dynamics of film flows*, Phys. Fluids 6, 1702 (1994).

[LSG] J. Liu, B. Schneider, J.P. Gollub *Three-dimensional instabilities of film flows*, Phys. Fluids 7, 55 (1995).

[NV] P. Noble, J.-P. Vila *Consistency, Stability, Gallilean indifference criteria for design of Two moments closure equations of Shallow water type for Thin Film laminar flow gravity driven.* in preparation.

[VL] B. Van Leer *Towards the ultimate conservative difference schemes: a second order sequel to Godunov's method* J. Comp. Phys 43 (1981) 357-372.

[T] E. Tadmor *Entropy stability theory for difference approximations of nonlinear conservation laws and related time-dependent problems* Acta Numerica (2003) pp. 451-512.